

Cross-Validation

Nipun Batra and teaching staff

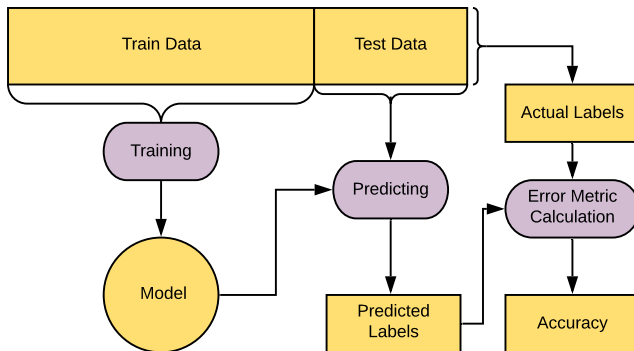
IIT Gandhinagar

August 1, 2025

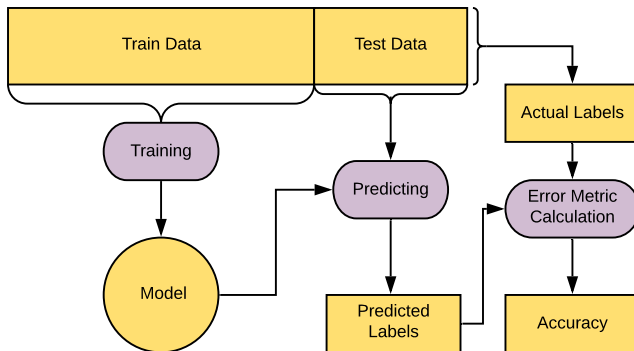
Outline

1. Introduction to Cross-Validation
2. Full Dataset Utilization
3. K-Fold Cross-Validation
4. Hyperparameter Optimization
5. Nested Cross-Validation
6. Cross-Validation Variants
7. Time Series Cross-Validation
8. Common Pitfalls and Best Practices
9. Summary and Key Takeaways

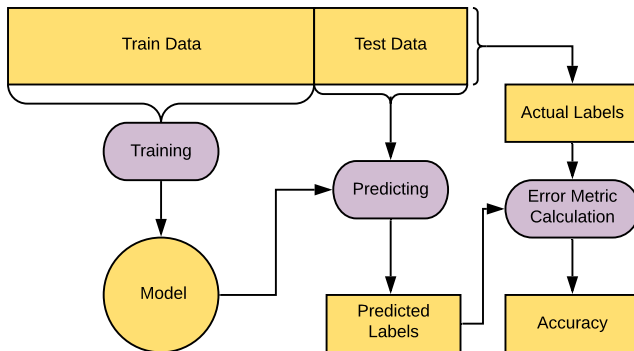
Our General Training Flow



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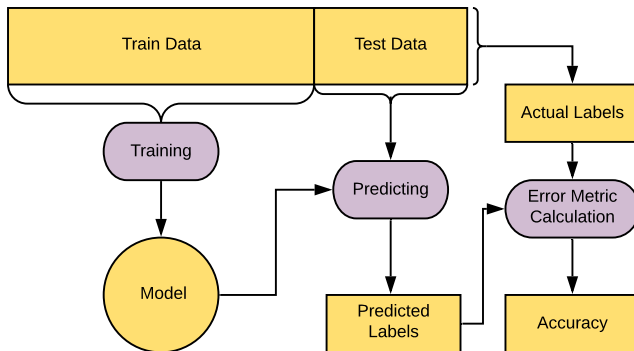


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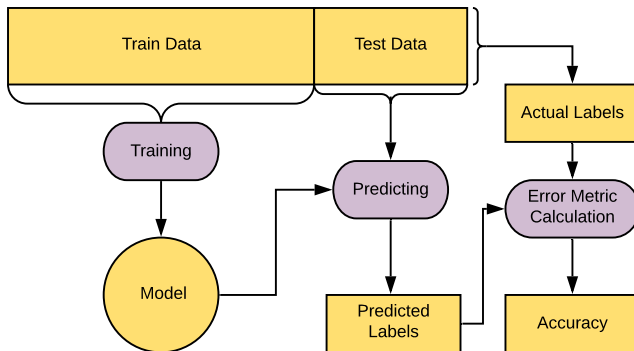
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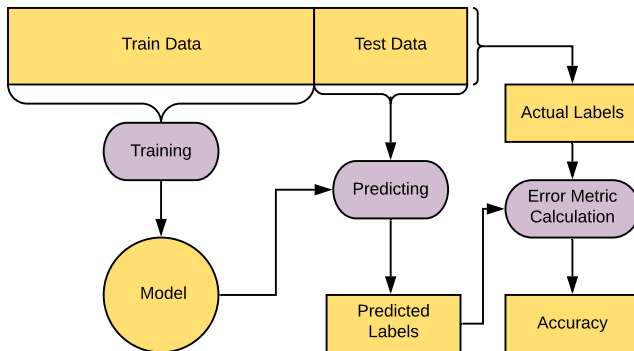
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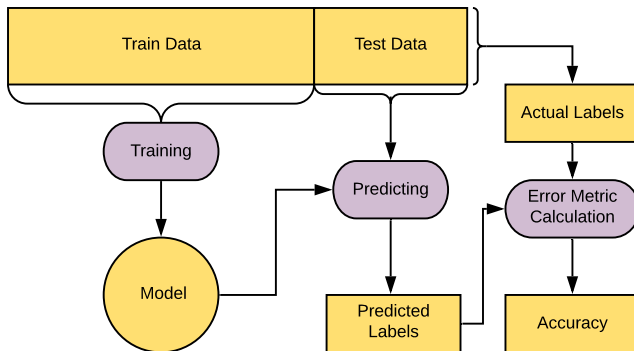
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Our General Training Flow



- Does not use the full dataset for training and does not test on the full dataset
- No way to optimize hyperparameters
- This simple train/test split has limitations we need to address

Pop Quiz #1

Question

What are the main limitations of using only a single train/test split?

Pop Quiz #2

Question

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Pop Quiz #3

Question

What are the main limitations of using only a single train/test split?

Answer

Pop Quiz #4

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training

Pop Quiz #5

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically

Pop Quiz #6

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Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen

Pop Quiz #7

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen
- May not get reliable performance estimates

How to use the full dataset for training?

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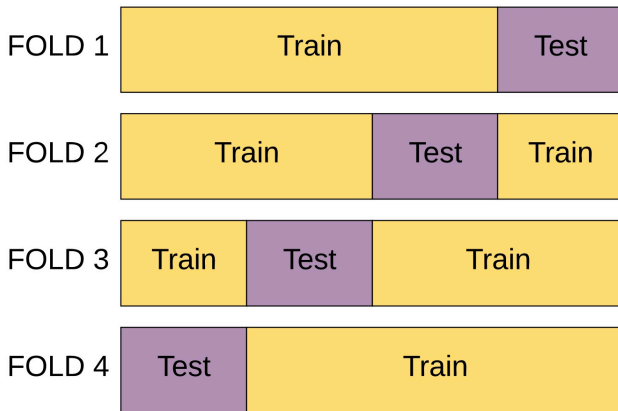
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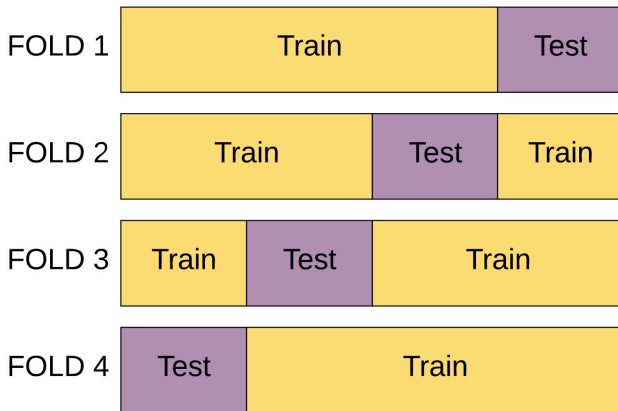
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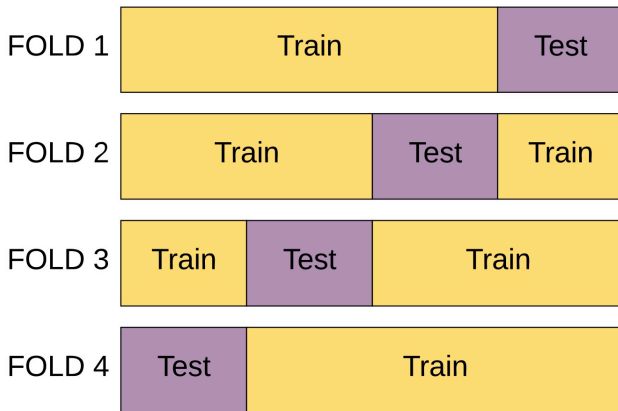
K-Fold Cross-Validation: Utilize Full Dataset for Testing



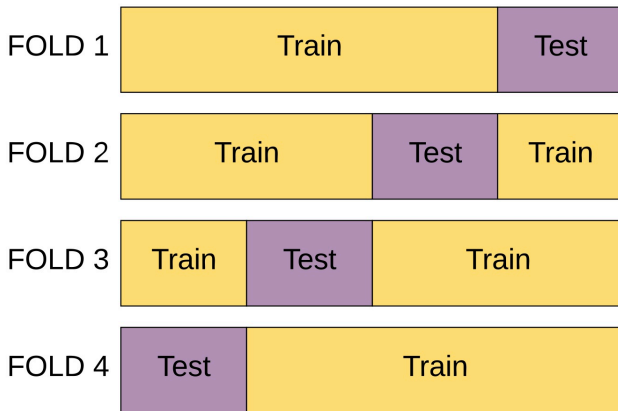
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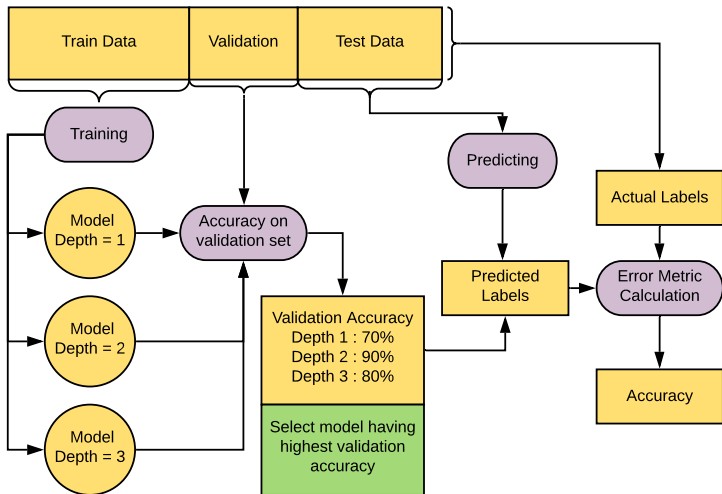
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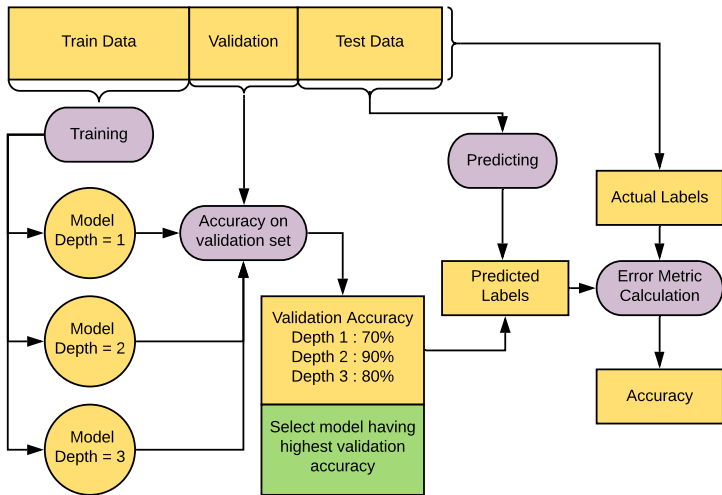
Answer

80 data points (4 out of 5 folds = $4/5 \times 100 = 80$)

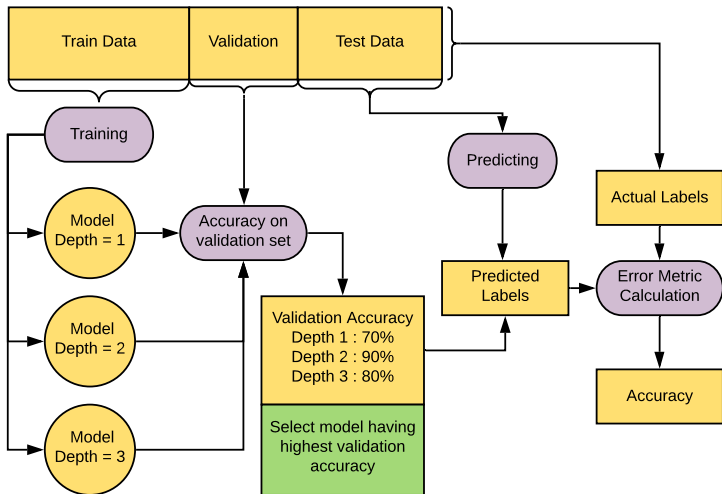
Optimizing Hyperparameters via the Validation Set



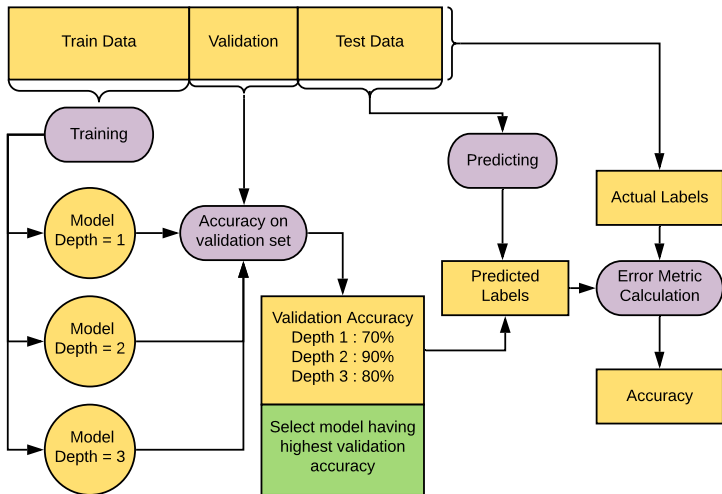
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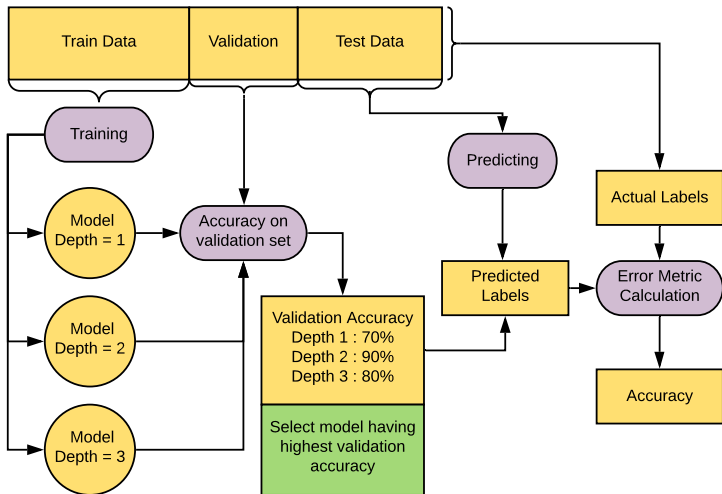
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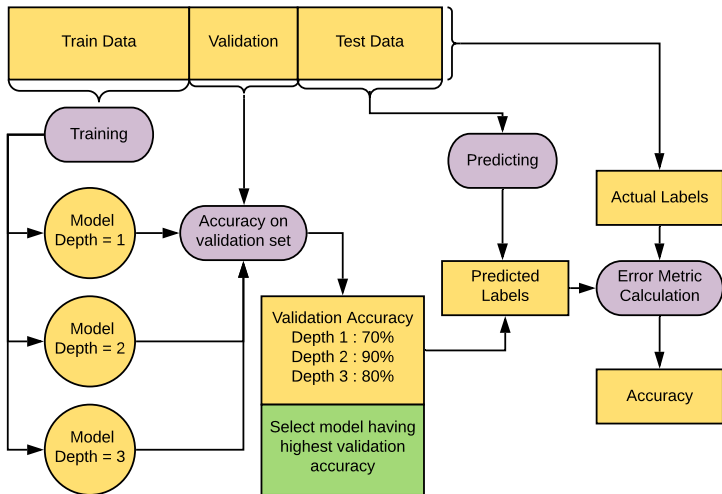
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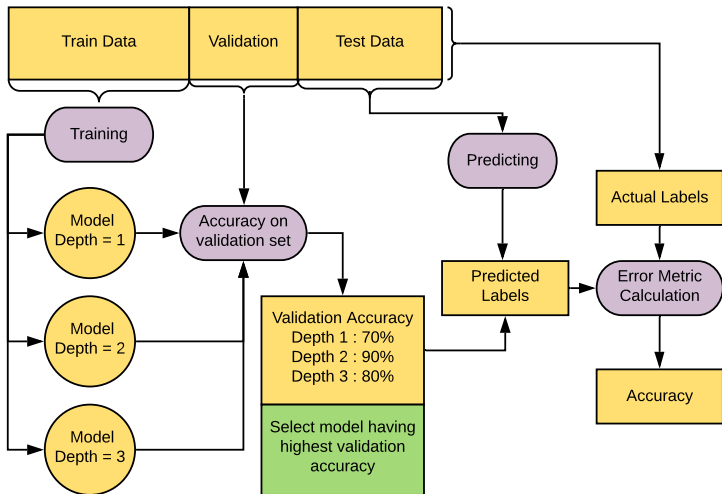
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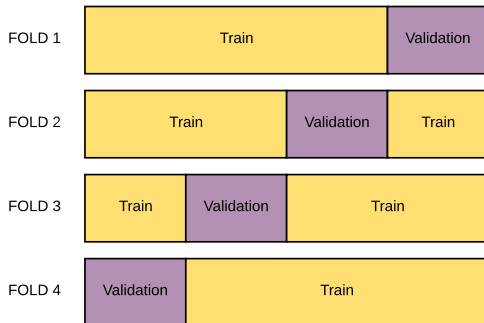


Nested Cross-Validation Process

Divide your training set into k equal parts.

Cyclically use 1 part as “validation set” and the rest for training.

Here $k = 4$

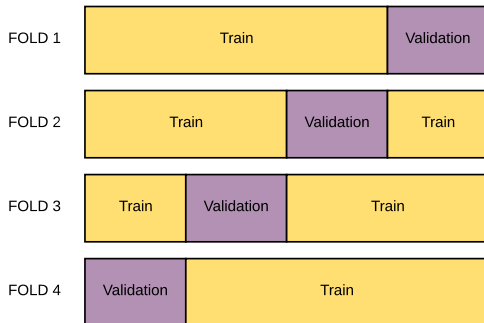


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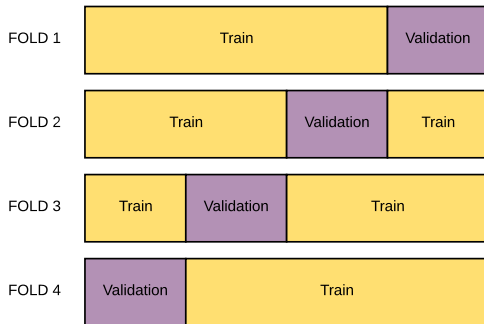


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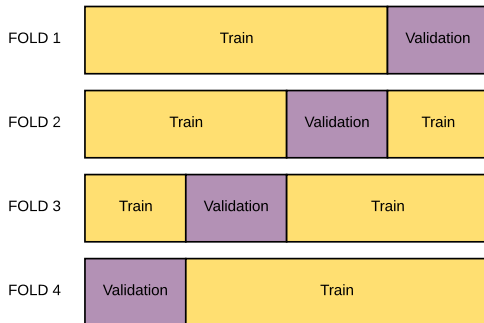
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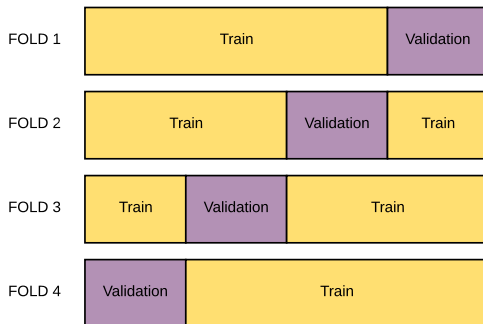
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- Process is systematic and exhaustive

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Pop Quiz #16

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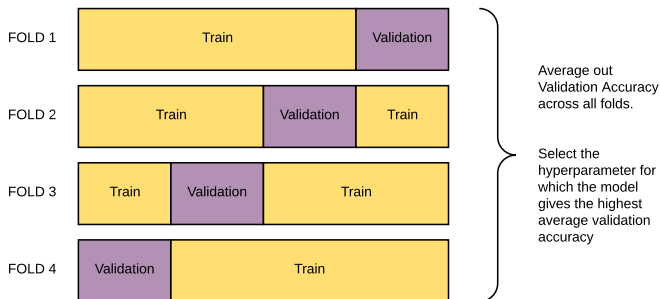
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Answer

- Simple CV: Used for model evaluation only
- Nested CV: Outer loop for model evaluation, inner loop for hyperparameter tuning
- Nested CV provides unbiased estimates when doing hyperparameter search

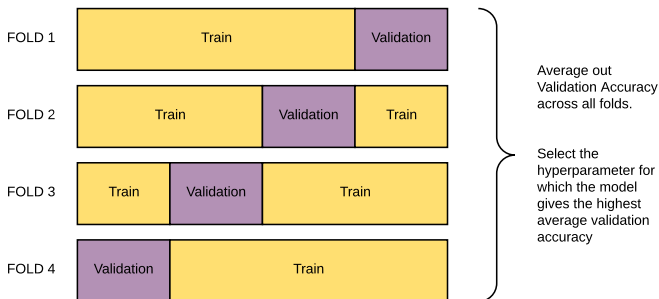
Cross-Validation Results

Average out the validation accuracy across all the folds
Use the hyperparameters with highest average validation accuracy



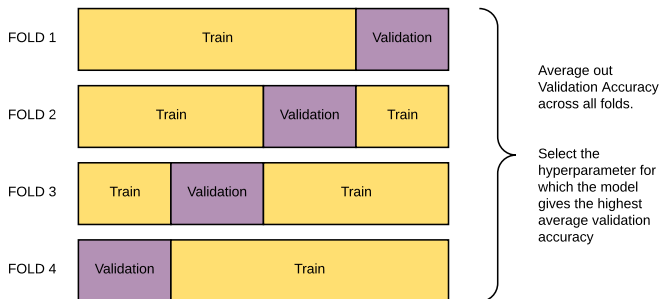
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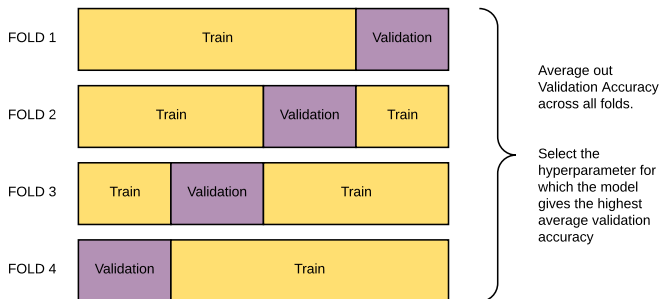
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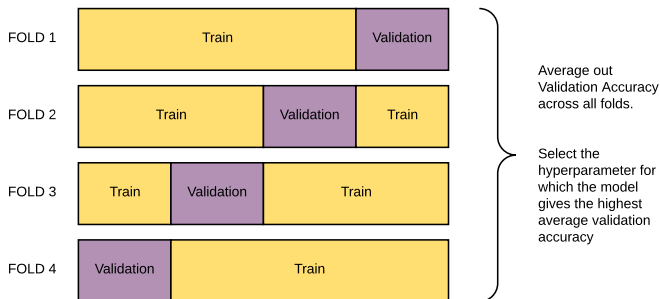
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- Standard deviation gives confidence in results

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- Standard deviation indicates reliability of the estimate

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Stratified Cross-Validation

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You have a binary classification dataset with 90% negative and 10% positive examples. Why is stratified cross-validation important here?

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- Stratified CV ensures each fold has $\sim 10\%$ positive examples
- Results in more reliable and consistent evaluation

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- Never use future data to predict past!

Common Cross-Validation Mistakes

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- **Incorrect Splitting:** Not accounting for grouped data
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- **Wrong Preprocessing:** Scaling on entire dataset before splitting
- **Ignoring Class Imbalance:** Not using stratified CV when needed

Pop Quiz #31

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Pop Quiz #32

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Pop Quiz #33

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Answer

Pop Quiz #34

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Answer

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Answer

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- Test fold statistics influence the training preprocessing

Pop Quiz #36

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Answer

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- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds

Pop Quiz #37

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Answer

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- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds
- Apply same transformation to corresponding test fold

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Answer

- This causes data leakage!
- Test fold statistics influence the training preprocessing
- Should compute statistics only on training folds
- Apply same transformation to corresponding test fold
- This gives more realistic performance estimates

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- **Model Comparison:** Fair comparison between different algorithms
- **Confidence Estimates:** Standard deviation indicates reliability

When to Use Different CV Types

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- **K-Fold (k=5,10):** General purpose, most common

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